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## Dynamic simulation of post-combustion capture system

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### Abstract

Post-combustion capture, as one of candidate technologies for carbon dioxide emission mitigation, has been employed in the chemical industry to separate CO<sub>2</sub> from a gas mixture. However, the largest CO<sub>2</sub> emission industry in China is the power industry, where CO<sub>2</sub> is mainly released from coal-fired power plants. The study on the dynamic simulation of post-combustion capture system is indispensable for the future implementation of post-combustion capture system on coal-fired power plants, because the output of each coal-fired power plant is controlled by the grid and varies with time in China. Using DYNOSIM software, we built a dynamic model for the typical post-combustion capture system, i.e. CO<sub>2</sub> absorption/desorption process using aqueous MEA solution. A set of case studies were carried out to investigate the performance of post-combustion capture system. The simulation results show that the flow rate of flue gas and the flow rate of lean solution can greatly influence the stability and the capture ratio of a post-combustion capture system. Therefore, some special control strategies should be designed for them in order to keep the capture system running steadily.

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*Keywords:* Dynamic model; Post-combustion capture; aqueous MEA solution; DYSIM; Coal-fired power plant

### 1. Introduction

China's energy is mainly provided by coal, which covered as much as 76.5% of China's primary energy consumption in 2010 [1]. Half of China's coal was used to produce electricity by coal-fired power plants. The total amount of electricity generated by coal-fired power plants was 3.21 trillion kWh in China in 2010 [2]. Calculated by the IPCC method and default emission factors [3], the estimated carbon dioxide emissions released by China's power industry were more than 3 billion tonnes in 2010.

Carbon capture and storage (CCS), as one of the potential technologies for carbon dioxide emission mitigation, has been developed in the past ten years. Post-combustion capture, one of the

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main carbon dioxide capture technologies, has shown its potential for commercial implementation, and several demonstrations have been established in coal-fired power plants in China [4]. However, the output of coal-fired power plant, which is controlled by the grid, varies with time in China, so the post-combustion capture system for a coal-fired power plant changes dynamically. The investigation on dynamic modeling of CO<sub>2</sub> capture system, as well as the coal-fired power plant, can provide quantitative simulation results to study the dynamic performance of CO<sub>2</sub> capture system and facilitate the CCS practice in the coal-fired power plant in China.

In the five-year Joint Work Plan of US-China CERC-ACTC<sup>†</sup> Program, a major task has been to perform a modeling and simulation study to determine the dynamic performance of the post-combustion capture system installed on the coal-fired power plant. The objective of the task is to build a set of dynamic models for coal-fired power plants with post-combustion capture system, investigate the operation and control characteristics of coal-fired power plants with post-combustion capture system, and provide technical insights for the development of low-carbon power generation. A dynamic model for post-combustion capture system was developed by Tsinghua University with the support of US-China CERC-ACTC Program. The preliminary simulation results of the dynamic model are shown in the paper.

## 2. Modeling approach

The post-combustion capture of CO<sub>2</sub> is a chemical absorption/stripping process, and a typical solution for it is the aqueous monoethanolamine (MEA) solution. Modeling and simulation with computer is a good choice for the performance study of the post-combustion capture system. Recently, the study on the dynamic modeling and simulation of post-combustion capture system has been performed by several researchers [5-9] via equilibrium or rate-based models. Lawal et al. [5,6] and Harun et al. [7] modeled the post-combustion CO<sub>2</sub> capture system on the gPROMS platform, Ziaii et al. [8] done his study basing on Aspen Custom Modeler, while Jayarathna et al. [9] developed a dynamic model in MATLAB. Though they selected different modeling platforms, the basic models for absorption/stripping process were similar. A few simulation tests had been done by them to study the dynamic performance of the capture system.

The software of DYNsIM, a state-of-the-art, field-proven dynamic process simulation program, is employed to model and simulate the absorption/stripping process using aqueous MEA solution in this work. In DYNsIM platform, we primitively build the post-combustion capture system with an absorber, a stripper, a reboiler and a heat exchanger. The diagram of the capture system process built in DYNsIM is shown as Fig. 1. The DYNsIM tower or column model, which would be used to simulate the absorber and stripper, use the equilibrium-based mass transfer approach. The acid-base equilibrium reactions, which take place in the absorber and stripper, are written as chemical dissociations following the approach of Kent and Eisenberg. The chemical equilibrium constants for the dissociation reactions are represented by polynomials in temperature. The non-ideality of the components would be ignored. The liquid enthalpy is calculated by adding a correction for the heat of reaction to the enthalpy calculated by the Ideal method. The vapor phase enthalpy, entropy and density are computed with the SRKM method. The liquid phase density is computed by the Ideal method.

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<sup>†</sup> CERC-ACTC: Clean Energy Research Center-Advanced Coal Technology Consortium. The primary purpose of CERC is to facilitate joint research, development, and commercialization of clean energy technologies between the U.S. and China. The Clean Coal, including Carbon Capture and Storage (CCS), is one of the three current CERC programs.

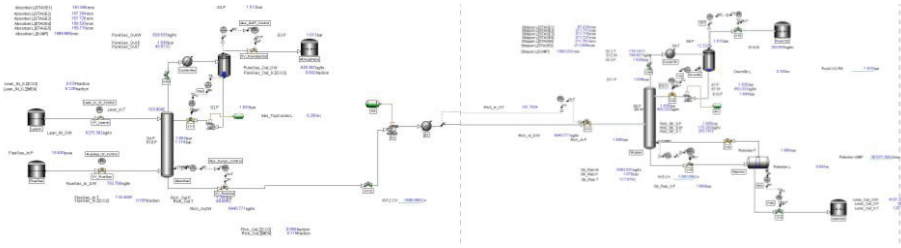


Fig. 1. Diagram of the capture system process

### 3. Model validation

A pilot plant facility was set up at the University of Texas at Austin [10], as a closed-loop absorption/stripping system for carbon dioxide removal from a flue gas. The absorber column and the stripper column of the pilot plant have the same size. Each column is a packed column with an inside diameter of 0.427 m and an approximate total height of 11.1 m. There are two packed bed sections with a height of 3.05 m in each column, so the total packing height of each column is 6.1 m. A collector plate and redistributors are installed between the two packed beds in order to uniformly redistribute the solution in the lower packed bed.

A pilot test using a 32.5 wt % aqueous MEA solution was performed in the pilot plant facility. 48 experimental cases at 24 different operating conditions were carried out in the test. We choose Case 47 as the reference steady state to validate our dynamic model built with DYNsIM. The actual operating conditions of Case 47 are presented in Table 1.

Table 1. The operation condition of Case 47 in [10]

Item	Value
Packing (Absorber/Stripper)	IMTP #40 / Flexipac 1Y
Lean Loading (mol CO <sub>2</sub> /mol MEA)	0.28
Mass -Inlet CO <sub>2</sub> (mol %)	12.7
Mole -Inlet CO <sub>2</sub> (mol %)	18
Gas Rate (Actual m <sup>3</sup> /min)	8.23
Liquid Rate (L/min)	30.1
CO <sub>2</sub> Removal (%)	69

The results of DYNsIM models are compared with the pilot test data of Case 47, as well as the Aspen steady-state simulation results [10]. Fig.1 and Fig. 2 show the temperature profiles of gas phase inside the absorber and the stripper of Case 47. Because of the reported inaccuracy in the flue gas flow measurement, the temperature value from the pilot research does not exactly match the value of simulation.

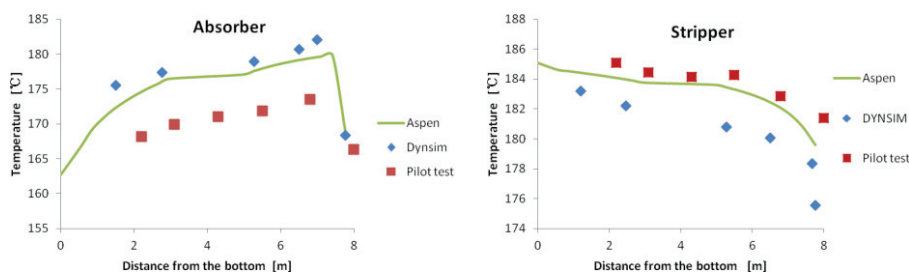


Fig. 2. Temperature profile of gas phase in (a) absorber and (b) stripper

#### 4. Case study

In order to achieve knowledge about the dynamic operation, the dynamic process of a post-combustion capture system was simulated and the dynamic behavior was analyzed by case studies in this work. In the case study, the operation condition was transiently changed when the post-combustion capture system was in a steady state, and the step response of the whole system was monitored until the system became steady again. Case 47 in [10] was chosen as the reference steady case, and all dynamic simulations started from it.

The change of the flow rate of flue gas and the flow rate of lean solution can greatly influence the behavior of capture system. Therefore, we made a stepwise change in the flow rate of flue gas and/or the flow rate of lean solution, while we kept all other parameters constant so as to avoid the disorder induced by the change of multiple parameters. The following simulations of dynamic scenarios were executed:

- Case 1: decreasing 20% of the flow rate of flue gas, i.e. increasing the liquid/gas ratio;
- Case 2: decreasing 20% of the flow rate of lean solution, i.e. reducing the liquid/gas ratio;
- Case 3: decreasing 20% of the flow rate of flue gas and lean solution simultaneously, i.e. keeping the liquid/gas ratio constant.

All the above step changes occurred when the steady state of capture system reached for 100 seconds.

The CO<sub>2</sub> capture rate, the rich loading and the gas phase temperature inside the stripper are focused upon to analyze the dynamic performance of the post-combustion capture system.

#### 5. Results and discussion

The dynamic model of post-combustion capture process using aqueous MEA solution was built in DYNsIM 4.5.4.11 and the dynamic cases were simulated on a Lenovo Thinkpad computer with two Intel Centrino 2.53 GHz processors.

##### 5.1. Case 1: Decreasing the flow rate of flue gas

The output of a real coal-fired power plant changes during a day in China, in order to meet the variation of electricity demand. Therefore, it is a common condition in a coal-fired power plant with CO<sub>2</sub> capture that the flow rate of flue gas varies with time. The dynamic behavior of the entire capture system in the condition should be study in order to develop a basic control strategy for the capture system.

In this case, the flow rate of flue gas instantly decreases from 0.133 m<sup>3</sup>/s to 0.106 m<sup>3</sup>/s after 100 seconds of steady state, i.e. a 20% reduction of the flow rate of flue gas. The dynamic simulation results are shown in Fig. 3 to Fig. 5, including the variation of rich loading with time, the variation of CO<sub>2</sub> capture ratio with time and the temperature profiles of gas phase inside the stripper at different time. We can find that it takes about 2000 seconds for the capture system to approach another steady state after the step change of the flow rate of flue gas. The flue gas entering the absorber reduces in the case, so the liquid/gas ratio increases. Therefore, the CO<sub>2</sub> capture ratio increases and a lower rich loading can meet the demand of CO<sub>2</sub> capture. Also the gas inside the stripper becomes hot, because the heat duty of reboiler keeps constant.

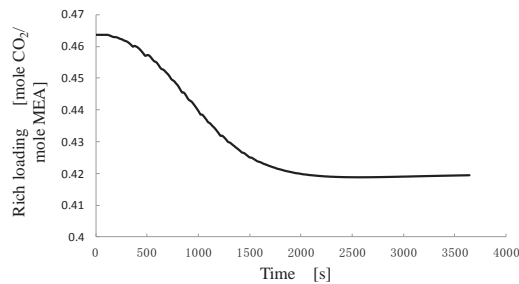


Fig. 3. Variation of rich loading with time

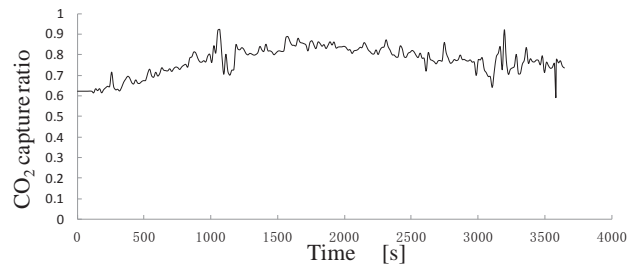


Fig. 4. Variation of CO<sub>2</sub> capture ratio with time

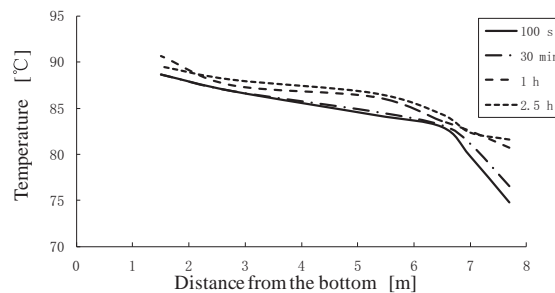


Fig. 5. Temperature profile of gas phase inside the stripper

5.2. Case 2: Decreasing the flow rate of lean solution

The flow rate of lean solution can be easily controlled to response the change of flue gas, comparing with other parameters, such as the temperature of lean solution, the lean loading, etc. Therefore, the dynamic behavior of the capture system induced by the step change of the flow rate of lean solution is studied in the case. The flow rate of lean solution instantly decreases from 0.5 L/s to 0.4 L/s after 100 seconds of steady state, i.e. a 20% reduction of the flow rate of lean solution. The dynamic simulation results are shown in Fig. 6 to Fig. 8. We can find that the capture system hardly approaches another steady state within 3600 seconds after the step change of the flow rate of lean solution. Though the flow rate of lean solution is reduced, there is only a little of increasing in the CO<sub>2</sub> capture ratio.

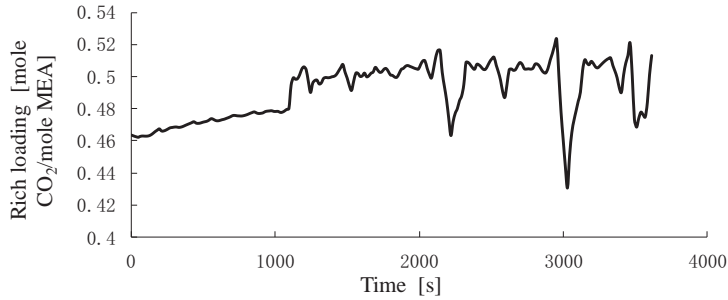


Fig. 6. Variation of rich loading with time

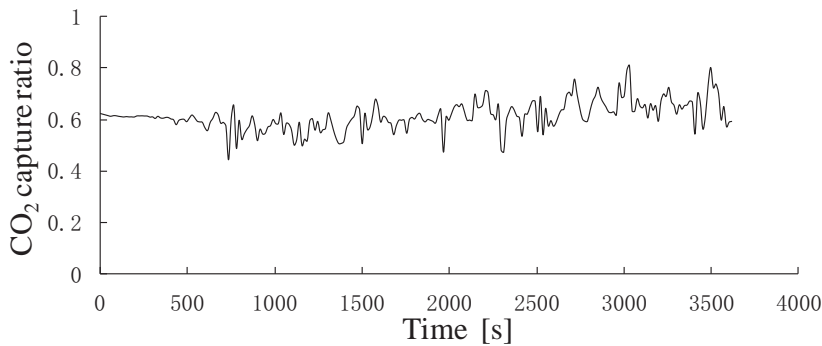


Fig. 7. Variation of CO<sub>2</sub> capture ratio with time

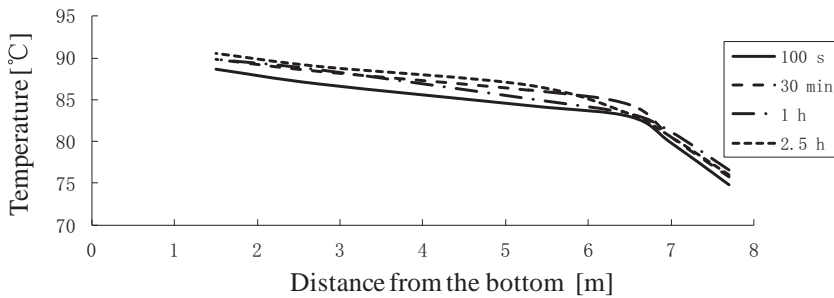


Fig. 8. Temperature profile of gas phase inside the stripper

### 5.3. Case 3: Decreasing the flow rate of flue gas but keeping L/G ratio constant

In this case, the flow rate of flue gas and the flow rate of lean solution change simultaneously. After 100 seconds of steady state, the flow rate of flue gas instantly decreases from  $0.133 \text{ m}^3/\text{s}$  to  $0.106 \text{ m}^3/\text{s}$ , and the flow rate of lean solution instantly decreases from  $0.5 \text{ L/s}$  to  $0.4 \text{ L/s}$  at the same time. The dynamic simulation results are shown in Fig. 9 to Fig. 11. We can find that it is easy for the capture system to approach another steady state in this case than in the above two cases. The  $\text{CO}_2$  capture ratio and the rich loading change a little.

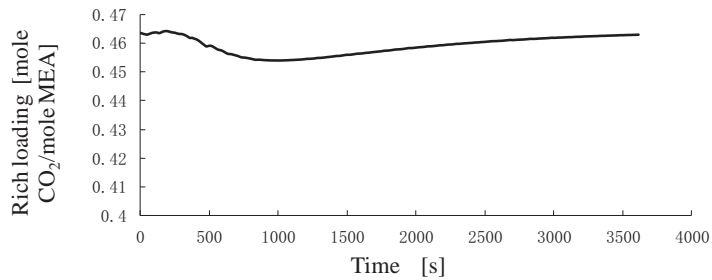


Fig. 9. Variation of rich loading with time

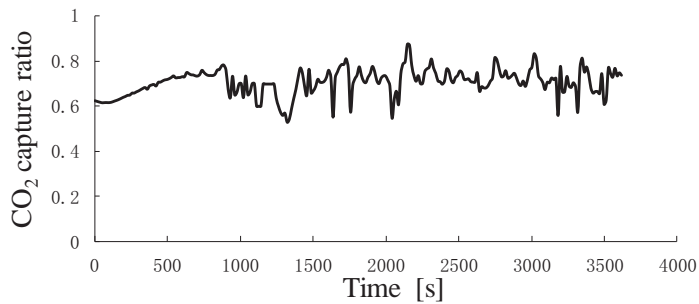


Fig. 10. Variation of  $\text{CO}_2$  capture ratio with time

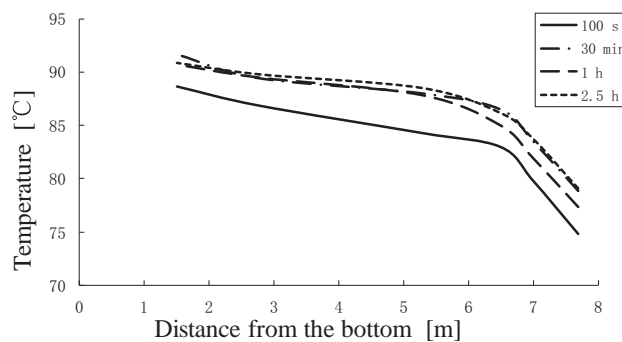


Fig. 11. Temperature profile of gas phase inside the stripper

## 6. Conclusion

Using DYN-SIM software, we develop a dynamic model for the post-combustion capture system. Some dynamic scenario cases are simulated with the model, and the dynamic performance of the post-combustion capture system is analyzed. The flow rate of flue gas and the flow rate of lean solution instantly change in the cases. The simulation results show that the flow rate of flue gas and the flow rate of lean solution can greatly influence the stability of the post-combustion capture system. Keeping a constant liquid/gas ratio can make the capture system running more fluently.

## Acknowledgements

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